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Variability of interlayer separation in SnSe thin films

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Abstract : SnSe has a sheet like orthorhombic structure with layers stacked along the c-axis, and the crystals can be easily cleaved in the ab-plane. Strong intralayer and very weak interlayer bonds give rise to a variability of the interlayer spacing. Hence, by using the variance and Fourier analysis of the X-ray diffraction line profiles the defect parameters and namely the mean fractional change in the interlayer spacings and its probability of occurrance have been calculated in case of SnSe thin films vacuum evaporated into mica substrates. Crystallite size, microstrain and dislocation densities have also been estimated. Effect of change in thickess of the films and increase in the substrate temperature during deposition has also been studied. Obtained results have been correlated with the photoconductivity of the films.

Keywords : Thin films, X-ray diffraction, interlayer separation

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Tin selenide has a highly anisotropic structure with tin selenide layers stacked along the c-axis and the crystals can easily be cleaved in the ab-plane. Tin selenide and its pseudobinary alloy, lead tin selenide is an important material for infrared opto-electronic devices [1]. Epitaxial structure and defects characterisation of tin selenide on alkali halides, PbSe, PbTe and SnTe have been reported in the literature [2,3]. In the present study, the X-ray diffraction technique has been choosen to investigate and information about crystallite size, microstrain, dislocation density, mean fractional change in the interlayer spacing and the probability of the planes having variability of interlayer spacing. Effect of deposition at higher substrate temperature has also been investigated. Similar studies of tin selenide thin films deposited on glass substrate have been reported earlier [4].

Assuming the X-ray diffraction line profile of tin selenide to be due to small particle size, strain and fault of the type of variable interlayer spacings, we have the second moment of the line profile W given by

$$W = W_p + W_S + W_D, \tag{1}$$

where W_P, W_S, W_D are the second moments of the three above effects repectively. Substitution of results available in the literature [5,6] gives

$$\frac{W}{\lambda}\frac{\cos\Phi}{(\Delta 2\Phi)} = \frac{1}{\pi^2 p'} + \frac{S\lambda}{(\Delta 2\Phi)\cos\Phi} \tag{2}$$

with

$$S = \frac{<e^2> - \beta_D^2/\pi^2}{d^2} \tag{3}$$

and

$$\frac{1}{p'} = \frac{1}{p'} + \frac{\beta_D}{d}. \tag{4}$$

$<e^2>$ = mean squared strain, $\beta_D = \gamma \sin^2 \pi\lambda g$,

d = mean interplanar spacing. ϕ = corresponding Bragg angle for wavelength, λ, p' = particle size, γ = probability of the reflecting planes having variable interlayer spacing, g = mean fractional change in interlayer spacing, $\Delta\ 2\phi$ = total range in 2ϕ scale over which the measurement are being made, 001 = the Miller indices of the reflecting planes modified by proper change of axes. Thus, a plot of $W\cos\phi/\lambda(\Delta 2\phi)$ against $\lambda\ /\ (\Delta 2\phi)\cos\phi$ will be linear and the slope will yield the value of $<e^2> - \beta_D^2/\pi^2$ and the intercept that of p'. The value of P in eq. 4 is determined from the initial slope of the $A(t)$ *vs* t curve where $A(t)$ is the real part of the t-th order Fourier tranform of the pure diffraction profile obtained by correcting the observed line profile for the geometrical effects by Stokes method [7]. Thus knowing the value of P', P and S from the variance and Fourier analysis, the values of $<e^2>^{1/2}$ and β_D can be obtained.

As shown by Wilson [8], the t-th order Fourier coefficient for layer defect is given by

$$A_d(t) = \exp(-2\beta_D t)\exp(-ibt) \tag{5}$$

where $b = \gamma \sin 2\pi lg$. Considering N terms of $A(t)$ and $B(t)$ the cosine and sine Fourier coefficients, the value of b is

$$b = \frac{1}{N}\sum_t \frac{1}{n}\frac{B(t)}{A(t)}. \tag{6}$$

Thus by knowing b and β_D, the value of γ and g are determined from the relations

$$g = \frac{1}{\pi}\tan^{-1}\frac{2\beta_D}{b} \tag{7}$$

and

$$\gamma = \frac{b}{\sin 2\pi g}. \tag{8}$$

Vacuum evaporated thin films of tin selenide of different thicknesses and various substrate temperatures were studied by the single line technique of [111] reflections only, since this was the only one reflection detectable on mica substrates. Studies were carried out with the help of Norelco X-ray diffractometer at scanning speed of 1/2 degree per minite by using monochromatic CuK_α radiations. Figure 1 shows the variation of $W \cos\phi/\lambda\sigma$ *versus*

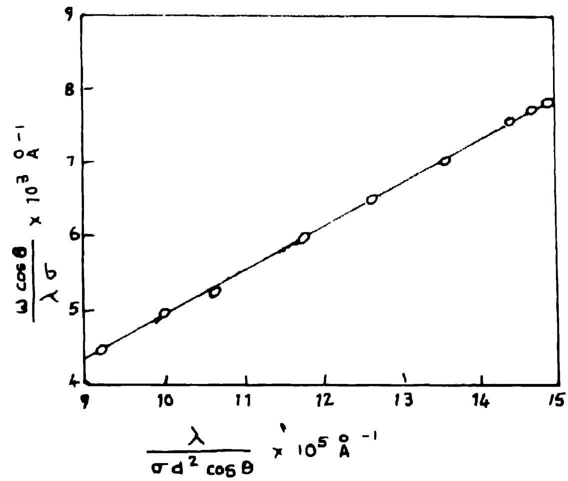

Figure 1. Variation of $W \cos\phi/\lambda\sigma$ *versus* $\lambda/\sigma d^2 \cos\phi$ variance W of the profile of SnSe film

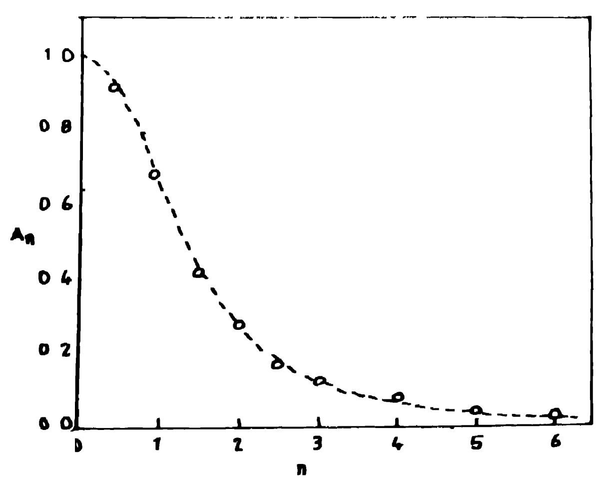

Figure 2. Variation of *A(n) versus (n)* of Fourier analysis of SnSe film.

$\lambda/\sigma d^2 \cos\phi$ of variance W of the line profile for [111] reflection of SnSe thin film deposited on mica substrate. Variation of *A(n) versus n* of Fourier analysis of tin selenide film have been shown in Figure 2. The experimental results are tabulated in Table 1.

It is observed that as the thickness of the thin film increases, the mean fractional change in interlayer spacing decreases, while its probability increases which means that more and more planes are being affected by such defects. The particle size increases with thickness of the film as well as substrate temperature whereas $<e^2>$ strain decreases with the same. These observations are similar to those reported by [9] on chemically deposited PbS films and

Table 1. Apparent crystalite size, strain, mean fractional change in interlayer spacing (g) and the probability of the reflecting planes having variability of interlayer spacing of SnSe thin films deposited on Mica Substrates

Sample No	Thickness nm	Substrate temp K	Apparent crystalite size (nm)	strain $/10^3$	g	γ
SS/1	100	302	31	3 16	0 88	0 02
SS/2	100	373	40	2.88	0 62	0 06
SS/3	200	302	67	1 93	0 73	0 14
SS/4	200	373	80	1 40	0 64	0 15

also to those of [10] on vacuum-deposited PbTe films. It is observed that with an increase in the temperature of deposition, there is a gradual increase in the crystallite size and the probability of the reflecting planes having variability of interlayer spacing, with a decrease in the strain value and a drastic fall in g the extent of the fault is also observed. Thus, we can infer that with an increase in the substrate temperature, the extent of the variability of interlayer spacing increases accompanied by the decrease in the microstrain, ultimately leading to the formation of new phase (at 472 K). With the formation of the new phase, there is a removal of faults in the crystallites of the low temperature phase. However as deposition at higher substrate temperatures occurs, possibly more microstrain and faults develop because of thermal expansion of the substrate and film. The extent of faults as given by g, decreases with the increase of thickness whereas the proportion of the planes affected, as given by the increase of v with the increase in the thickness of the films. Similar observations have been reported by Chaudhuri *et al* [11] for the case of tellunium films. It is observed that in the case of thin films, the extent of fault being greater, the strain is low, whereas in the case of thick films, fault is small and the strain is large. Deposition at higher substrate temperature gives crystallites of larger dimensions. Thus, the fault is relatively high and strain is also more. For all the films, it is observed that small crystallites are accompanied by greater faults and small strains. Finally, photosensitivity was found to decrease with the increase in the crystallite size values.

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